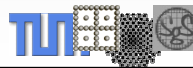


Continuous Models 2: PDE

- so far: only time as independent variable
- ODE-based population models sometimes too coarse:
 - population in the USA during California gold rush in the 1850s
 - predictions of the UN concerning world population (industrialized countries versus third world)
- therefore: suppose $p(x,t)$ or $p(x,y,t)$ instead of $p(t)$
 - California gold rush: 1D sufficient (east-west)
 - world population: perhaps 1D (north-south), perhaps 2D
- taking space into account makes models
 - more accurate (spatial effects are no longer neglected)
 - more complicated (analytical solution becomes harder, numerical solution means a lot of additional work)
- standard example: heat conduction



Introduction to Scientific Computing
Lesson 5: Continuous Models (PDE)



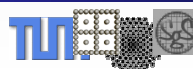
Slide 1

Modelling with PDE

- taking space into account is typical for many problems or phenomena from physics or continuum mechanics:
 - fluid mechanics: where will we get a tornado?
 - structural mechanics: where will be the crack?
 - process engineering: where is it how hot in the reactor?
 - electromagnetism: where is which electron density?
 - geology: where will the earthquake happen?
- more independent variables entail *partial* derivatives
- we distinguish:
 - *stationary* problems: no time-dependence
 - *unsteady* problems: time-dependence (perhaps, but not necessarily, with a stationary limit for increasing time)



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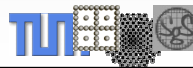
Slide 2

Heat Conduction

- central problem of thermodynamics
- let heat affect an object's boundary – propagation?
 - a wire, heated at one end
 - a metal plate, heated at one side
 - water cooling the reactor in a nuclear power plant
 - a room in winter: where to place the heating
 - a room in summer: effect of direct sunshine
 - boiling water in a pot on a ceramic hob
- central function of interest: temperature T
 $T(x;t)$ or $T(x, y;t)$ or $T(x, y, z;t)$
- The values of T will depend on the material and its heat conductivity.



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Slide 3

Modelling Heat Conduction 1

- part 1 of the model: the PDE, indicating the relations of changes of T with respect to time and space (3D):

$$\kappa \cdot (T_{xx} + T_{yy} + T_{zz}) = \kappa \cdot \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) = \frac{\partial T}{\partial t} = T_t$$

or shortly $\kappa \cdot \Delta T = T_t$ with the Laplace operator Δ

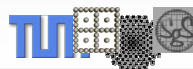
- short derivation (excursion to physics):
 - starting point is the basic principle of energy conservation
 - changes of heat in some part D of our domain are due to flux in/out D 's surface and to external sources and drains in D

$$\frac{\partial}{\partial t} \int_D \rho c T dV = \int_D q dV + \int_{\partial D} k \nabla T \cdot \vec{n} dS$$

- density ρ , specific heat c , external term q , heat conductivity k , outer normal vector, n volume/surface element dV/dS



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Slide 4

Modelling Heat Conduction 2

➤ derivation of the heat equation (continued):

- transform the above equation according to Gauß' theorem:

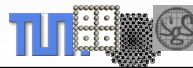
$$\int_D (\rho c T_t - q - k \Delta T) dV = 0$$

- This holds for an arbitrary part D of our domain. Hence, the integrand must vanish:

$$T_t = \kappa \Delta T + \frac{q}{\rho c}, \quad \kappa = \frac{k}{\rho c}$$

- $\kappa > 0$ is called the *thermal diffusion coefficient* (since the Laplace operator stands for a (heat) diffusion process)
- For vanishing external influence $q=0$, we get (and, thus, have derived) the famous **heat equation**:

$$T_t = \kappa \Delta T$$



Modelling Heat Conduction 3

➤ part 2 of the model: the PDE needs **boundary** or **initial-boundary** conditions to provide a unique solution:

- Dirichlet** boundary conditions: fix T on (part of) the boundary

$$T(x, y, z) = \varphi(x, y, z)$$

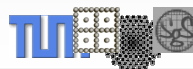
- Neumann** boundary conditions: fix T's normal derivative on (part of) the boundary:

$$\frac{\partial T}{\partial n}(x, y, z) = \varphi(x, y, z)$$

- pure Dirichlet and mixtures are allowed, pure Neumann b.c. do not lead to a unique solution (with T solves T+constant the PDE, too)

- in case of time-dependence: initial conditions for $t=0$

➤ in case of no time-dependence: Laplace equation



Modelling Heat Conduction 4

➤ meaning of boundary conditions:

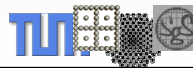
- **Dirichlet**: the temperature T is prescribed itself along (part of) the boundary (some defined heating or cooling)
- **Neumann**: the temperature flux through (part of) the boundary is prescribed (if vanishing: complete isolation, no orthogonal transport of heat into or out of the domain)

➤ analytical solutions:

- In simple (1D) configurations, solutions can be given explicitly via *separation of variables* (*Fourier's method*). We will discuss these in the exercises.
- The heat equation is a simple case of a PDE, where general statements concerning existence and uniqueness of solutions are possible. Often, such theorems can not be proven.



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Slide 7

Types of PDE

➤ The heat equation is a *linear PDE of second order*:

$$\sum_{i,j=1}^d a_{i,j}(\vec{x}) \cdot u_{x_i, x_j}(\vec{x}) + \sum_{i=1}^d a_i(\vec{x}) \cdot u_{x_i}(\vec{x}) + a(\vec{x}) \cdot u(\vec{x}) = f(\vec{x})$$

➤ three types are distinguished:

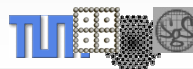
- **elliptic** PDE: the matrix A of the $a_{i,j}$ is pos. or neg. definite
- **parabolic** PDE: one eigenvalue of A is zero, the others have the same sign, and the rank of A together with the vector of the a_i is full (d)
- **hyperbolic** PDE: A has 1 pos. and $d-1$ neg. eigenvalues or vv.

➤ examples:

- elliptic: Laplace equation $\Delta u = 0$
- parabolic: heat equation $\Delta u = u_t$
- hyperbolic: wave equation $\Delta u = u_{tt}$



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Slide 8